w3-03

FILE 'HOME' ENTERED AT 12:32:06 ON 03 JUN 2003

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:32:15 ON 03 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2
DICTIONARY FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

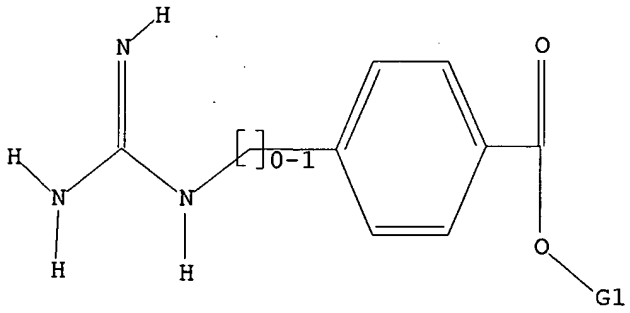
Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 09975136 before allowance.str

L1 STRUCTURE UPLOADED

=> id l1
COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by
structure-building or screen commands and text search terms. L#s
created via the STRUCTURE or SCREEN commands must be searched in the
structures files separately from text terms or profiles. The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

```
=> search l1 sss sam
SAMPLE SEARCH INITIATED 12:32:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    208 TO ITERATE

100.0% PROCESSED     208 ITERATIONS                          50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

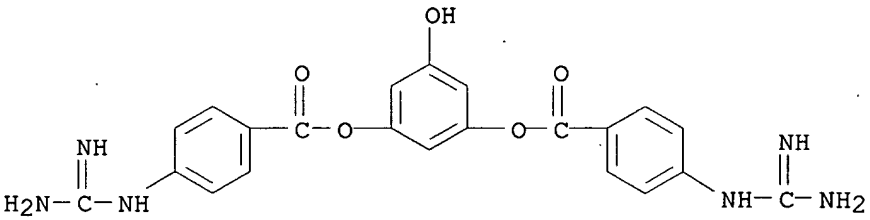
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          3295 TO     5025
PROJECTED ANSWERS:             1047 TO     2113

L2           50 SEA SSS SAM L1

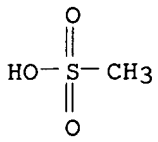
=> d scan

L2   50 ANSWERS   REGISTRY  COPYRIGHT 2003 ACS
IN   Benzoic acid, 4-[(aminoiminomethyl)amino]-, 5-hydroxy-1,3-phenylene
ester,
     dimethanesulfonate (salt) (9CI)
MF   C22 H20 N6 O5 . 2 C H4 O3 S

     CM   1
```

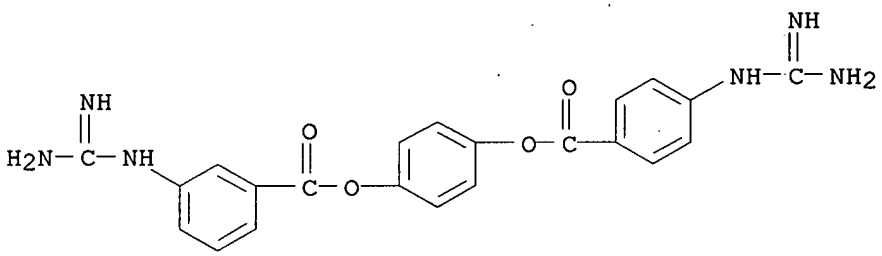


```
     CM   2
```



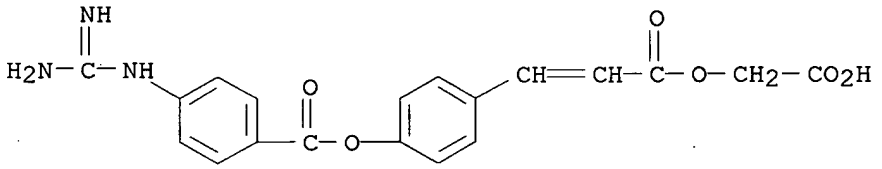
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 3-[(aminoiminomethyl)amino]-, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]phenyl ester (9CI)
MF C22 H20 N6 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[3-(carboxymethoxy)-3-oxo-1-propenyl]phenyl ester (9CI)
MF C19 H17 N3 O6
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

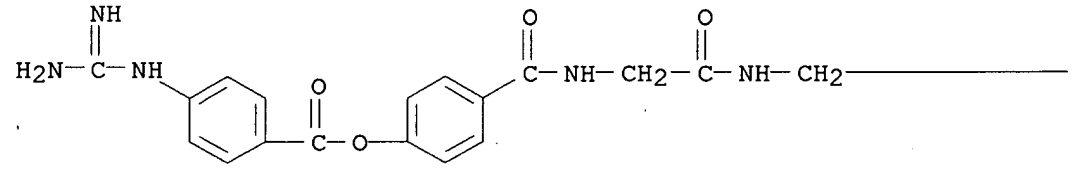
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Poly(oxy-1,2-ethanediyl), .alpha.-[2-[[[[4-[[4-

[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino]acetyl]amino]ethyl}-
.omega.-methoxy-, monomethanesulfonate (9CI)

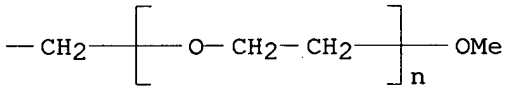
MF (C2 H4 O)n C20 H23 N5 O5 . C H4 O3 S

CM 1

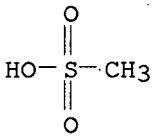
PAGE 1-A



PAGE 1-B



CM 2

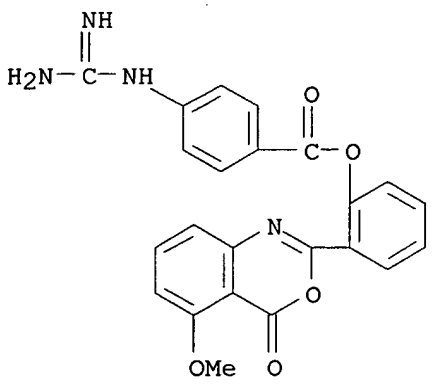


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

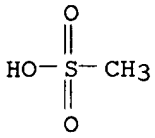
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-(5-methoxy-4-oxo-4H-3,1-
benzoxazin-2-yl)phenyl ester, monomethanesulfonate (9CI)

MF C23 H18 N4 O5 . C H4 O3 S

CM 1

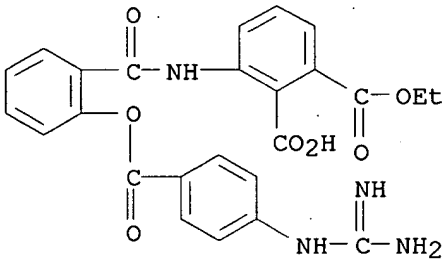


CM 2

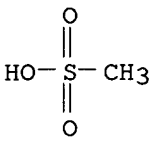


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1,2-Benzenedicarboxylic acid,
3-[[2-[[4-[(aminoiminomethyl)amino]benzoyl]o
xy]benzoyl]amino]-, 1-ethyl ester, monomethanesulfonate (9CI)
MF C25 H22 N4 O7 . C H4 O3 S

CM 1



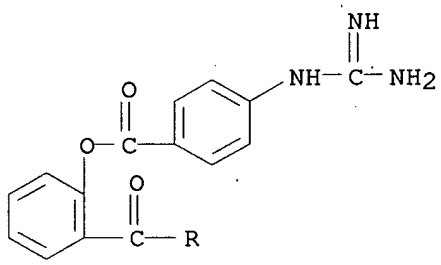
CM 2

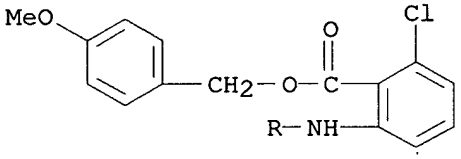


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

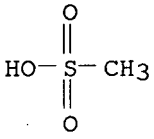
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid,
2-[[2-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino
]-6-chloro-, (4-methoxyphenyl)methyl ester, monomethanesulfonate (9CI)
MF C30 H25 Cl N4 O6 . C H4 O3 S

CM 1

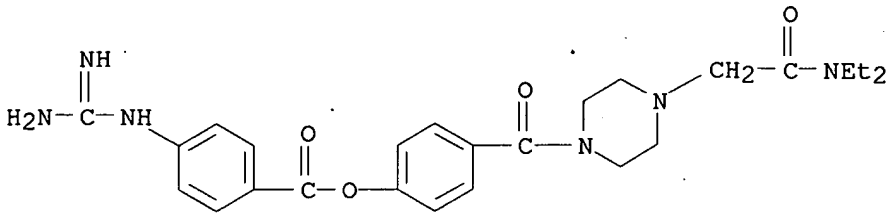




CM 2



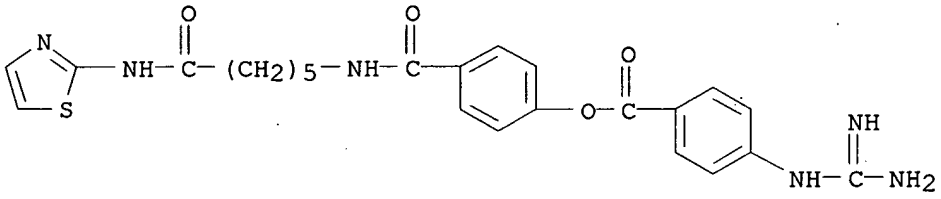
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[4-[2-(diethylamino)-2-
oxoethyl]-1-piperazinyl]carbonyl]phenyl ester (9CI)
MF C25 H32 N6 O4
CI COM



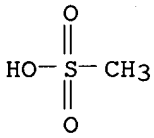
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[[6-oxo-6-(2-thiazolylamino)hexyl]amino]carbonyl]phenyl ester, monomethanesulfonate (9CI)
MF C24 H26 N6 O4 S . C H4 O3 S

CM 1

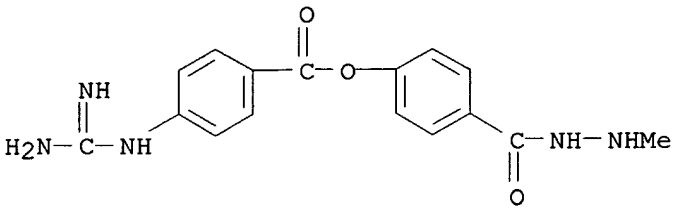


CM 2

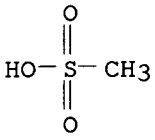


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[(2-methylhydrazino)carbonyl]phenyl ester, monomethanesulfonate (9CI)
MF C16 H17 N5 O3 . C H4 O3 S

CM 1

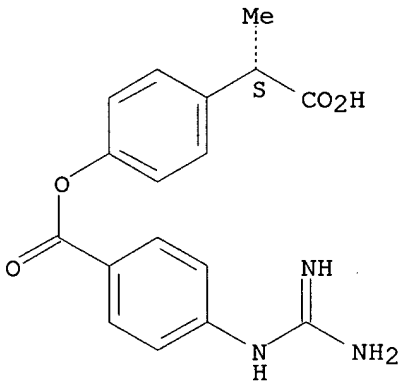


CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, (S)- (9CI)
MF C17 H17 N3 O4
CI COM

Absolute stereochemistry.

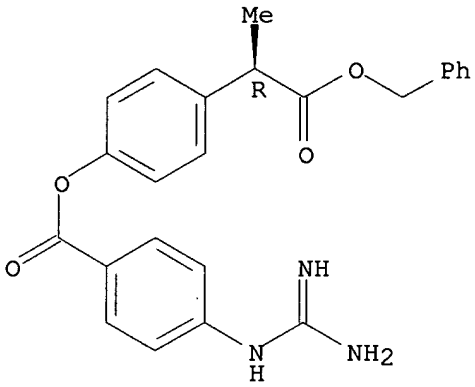


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

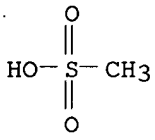
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, phenylmethyl ester, (R)-, monomethanesulfonate (9CI)
MF C24 H23 N3 O4 . C H4 O3 S

CM 1

Absolute stereochemistry.

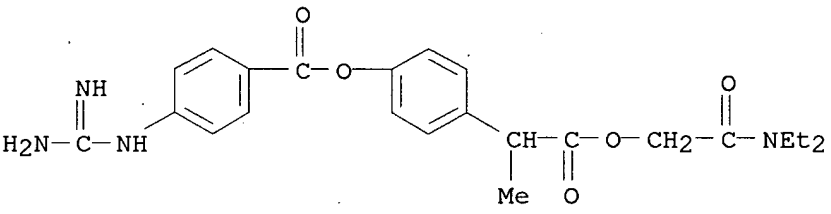


CM 2

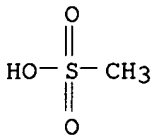


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 2-(diethylamino)-2-oxoethyl ester, monomethanesulfonate (9CI)
MF C23 H28 N4 O5 . C H4 O3 S

CM 1

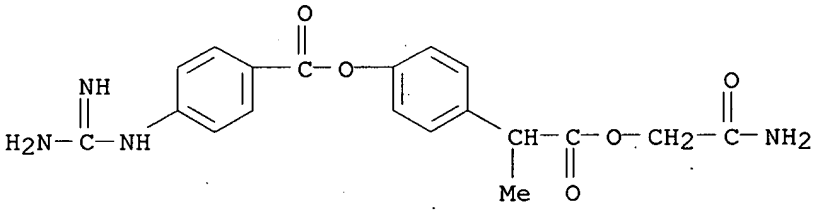


CM 2

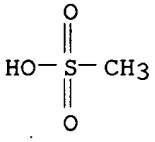


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 2-amino-2-oxoethyl ester, monomethanesulfonate (9CI)
MF C19 H20 N4 O5 . C H4 O3 S

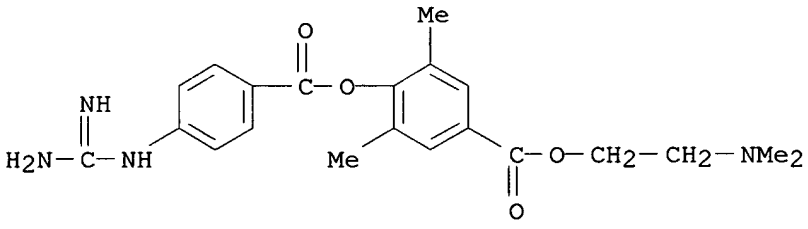
CM 1



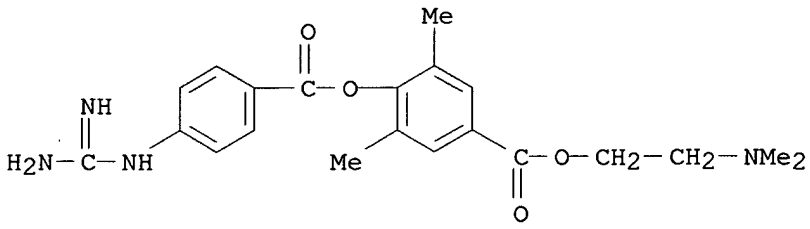
CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-3,5-dimethyl-, 2-(dimethylamino)ethyl ester, dihydrochloride (9CI)
MF C21 H26 N4 O4 . 2 Cl H



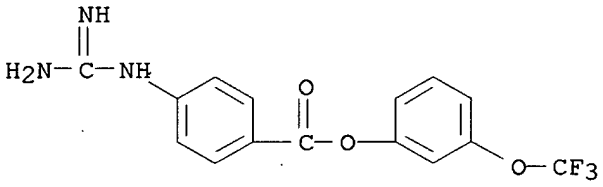
●2 HCl



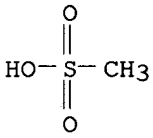
●2 HCl

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 3-(trifluoromethoxy)phenyl ester, monomethanesulfonate (9CI)
MF C15 H12 F3 N3 O3 . C H4 O3 S

CM 1

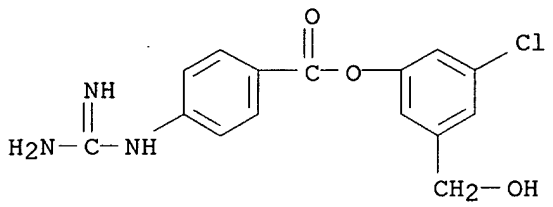


CM 2

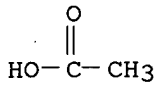


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 3-chloro-5-(hydroxymethyl)phenyl ester, monoacetate (salt) (9CI)
MF C15 H14 Cl N3 O3 . C2 H4 O2

CM 1

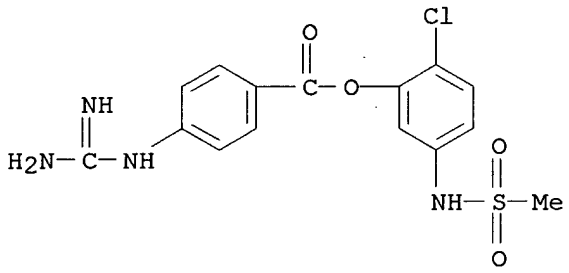


CM 2

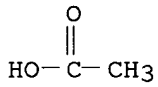


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-chloro-5-[(methylsulfonyl)amino]phenyl ester, monoacetate (9CI)
MF C15 H15 Cl N4 O4 S . C2 H4 O2

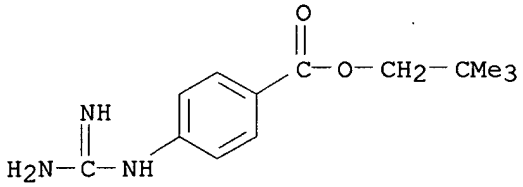
CM 1



CM 2



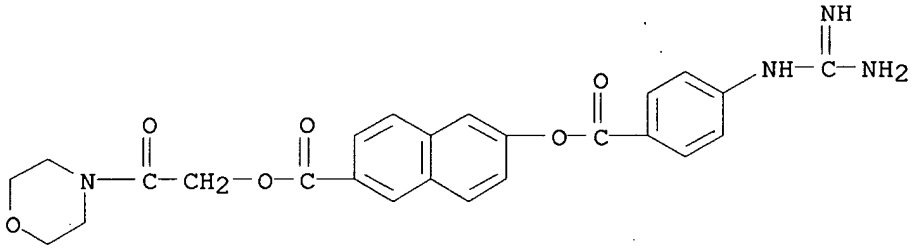
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester (9CI)
MF C13 H19 N3 O2



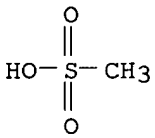
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Naphthalenecarboxylic acid,
6-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-
, 2-(4-morpholinyl)-2-oxoethyl ester, monomethanesulfonate (9CI)
MF C25 H24 N4 O6 . C H4 O3 S

CM 1

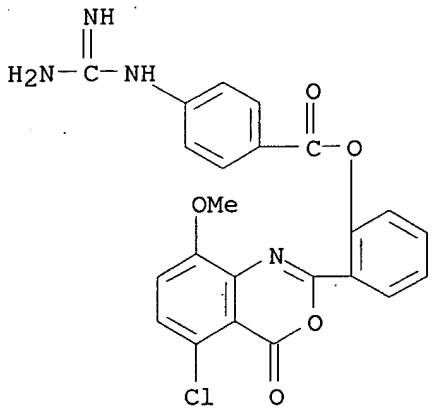


CM 2

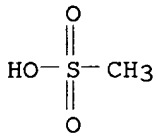


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,
2-(5-chloro-8-methoxy-4-oxo-4H-
3,1-benzoxazin-2-yl)phenyl ester, monomethanesulfonate (9CI)
MF C23 H17 Cl N4 O5 . C H4 O3 S

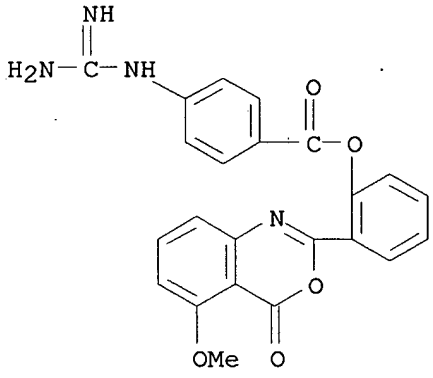
CM 1



CM 2

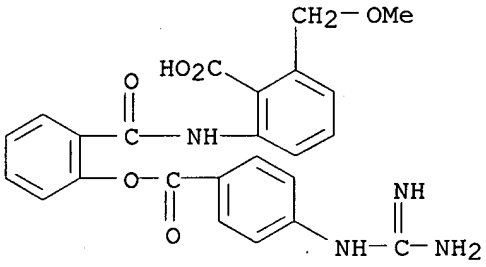


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-(5-methoxy-4-oxo-4H-3,1-benzoxazin-2-yl)phenyl ester (9CI)
MF C23 H18 N4 O5
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

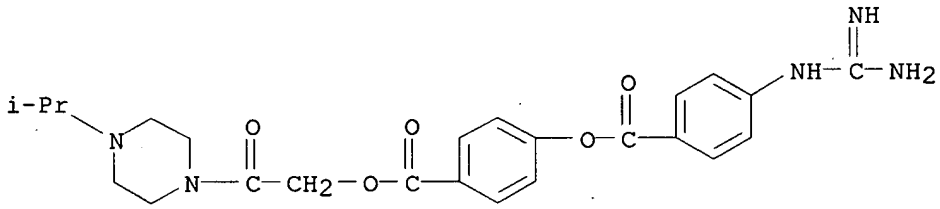
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid,
2-[[2-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino
    ]-6-(methoxymethyl)- (9CI)
MF C24 H22 N4 O6
CI COM



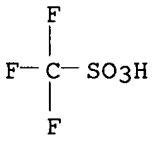
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[2-[4-(1-methylethyl)-1-
    piperazinyl]-2-oxoethoxy]carbonyl]phenyl ester,
    mono(trifluoromethanesulfonate) (9CI)
MF C24 H29 N5 O5 . C H F3 O3 S

    CM 1

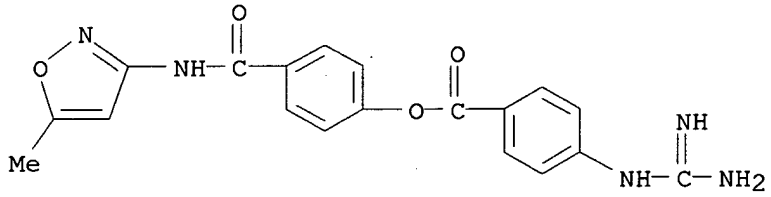


    CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[(5-methyl-3-isoxazolyl)amino]carbonyl]phenyl ester, monomethanesulfonate (9CI)
MF C19 H17 N5 O4 . C H4 O3 S

CM 1



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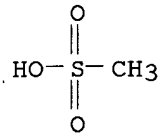
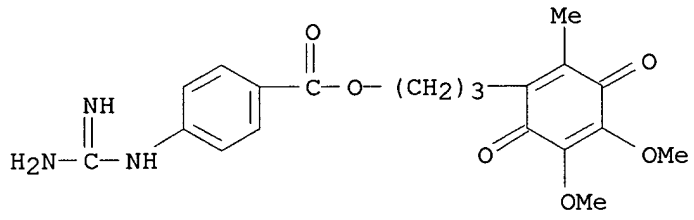


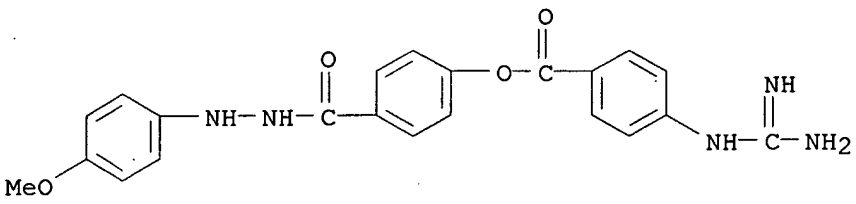
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 3-(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)propyl ester (9CI)
MF C20 H23 N3 O6



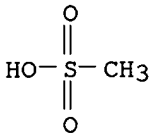
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[2-(4-methoxyphenyl)hydrazino]carbonyl]phenyl ester, monomethanesulfonate (9CI)
MF C22 H21 N5 O4 . C H4 O3 S

CM 1

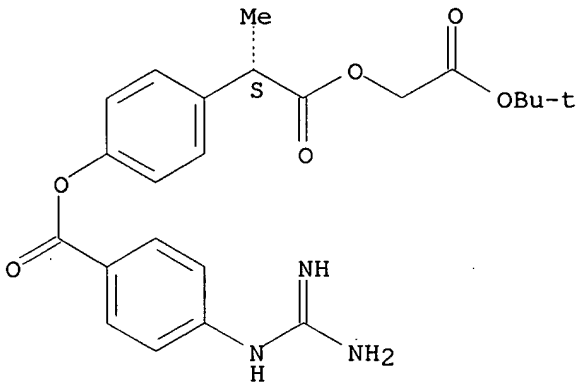


CM 2



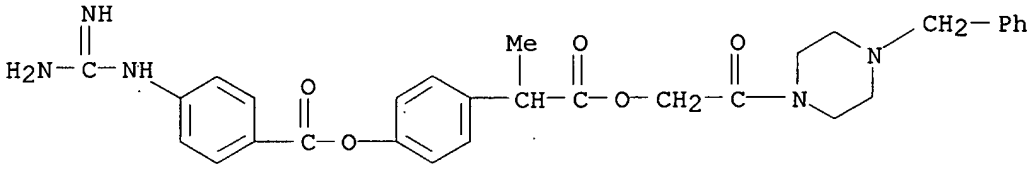
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 2-(1,1-dimethylethoxy)-2-oxoethyl ester, (S)- (9CI)
MF C23 H27 N3 O6
CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

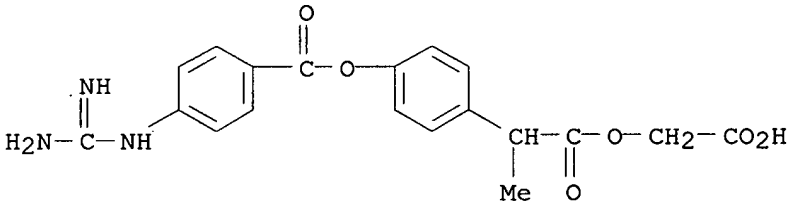
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 2-oxo-2-[4-(phenylmethyl)-1-piperazinyl]ethyl ester (9CI)
MF C30 H33 N5 O5
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, carboxymethyl ester, monomethanesulfonate (9CI)
MF C19 H19 N3 O6 . C H4 O3 S

CM 1



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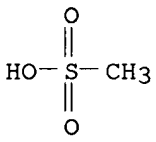
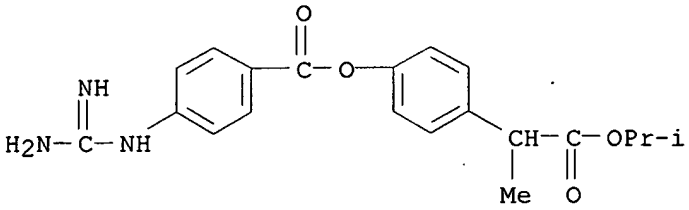


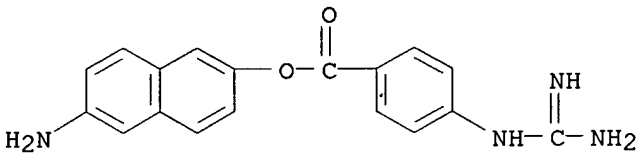
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 1-methylethyl ester (9CI)
MF C20 H23 N3 O4
CI COM



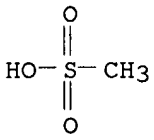
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 6-amino-2-naphthalenyl ester, dimethanesulfonate (9CI)
MF C18 H16 N4 O2 . 2 C H4 O3 S

CM 1



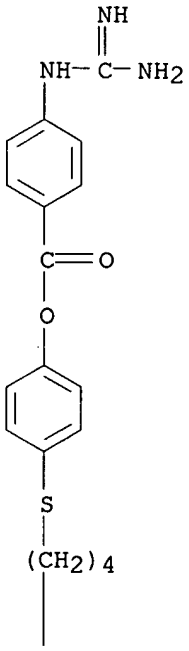
CM 2



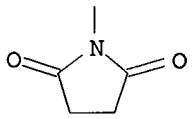
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[4-(2,5-dioxo-1-pyrrolidinyl)butyl]thio]phenyl ester, monomethanesulfonate (9CI)
MF C22 H24 N4 O4 S . C H4 O3 S

CM 1

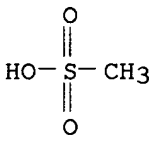
PAGE 1-A



PAGE 2-A



CM 2

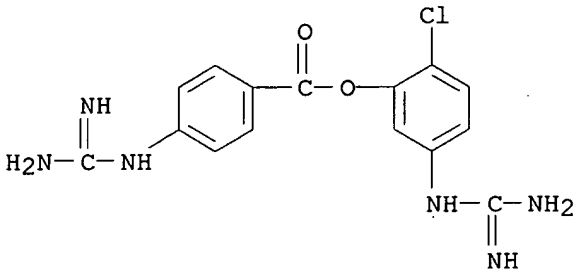


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 5-[(aminoiminomethyl)amino]-2-chlorophenyl ester, diacetate (9CI)

MF C15 H15 Cl N6 O2 . 2 C2 H4 O2

CM 1



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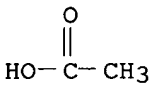
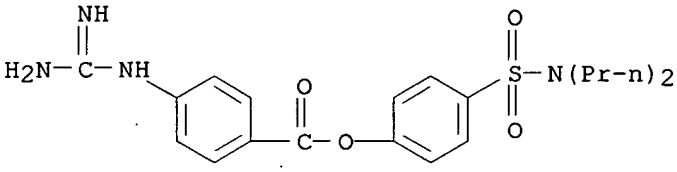


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[(dipropylamino)sulfonyl]phenyl ester, monomethanesulfonate (9CI)
MF C20 H26 N4 O4 S . C H4 O3 S

CM 1



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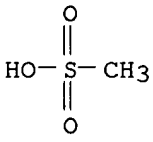
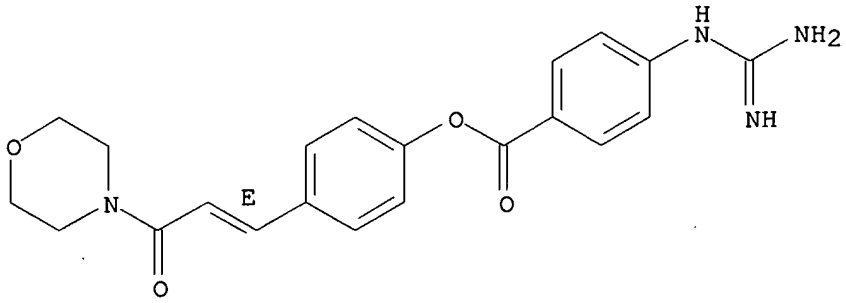


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[(1E)-3-(4-morpholinyl)-3-oxo-1-propenyl]phenyl ester (9CI)
MF C21 H22 N4 O4
CI COM

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):o
'O' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> search l1 sss full
FULL SEARCH INITIATED 12:34:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3885 TO ITERATE

100.0% PROCESSED 3885 ITERATIONS 1258 ANSWERS
SEARCH TIME: 00.00.01

L3 1258 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	149.75	149.96

FILE 'CAPLUS' ENTERED AT 12:34:57 ON 03 JUN 2003

FILE COVERS 1907 - 3 Jun 2003 VOL 138 ISS 23
FILE LAST UPDATED: 2 Jun 2003 (20030602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l3
L4 876 L3

=> ?bact?
L5 613320 ?BACT?

=> l4 and l5
L6 31 L4 AND L5

=> d l6 20-31 ti

L6 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Probiotics: antistaphylococcal activity of 4-aminocyclohexanecarboxylic acid, aminobenzoic acid, and their derivatives and structure-activity relations

L6 ANSWER 21 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Cephalosporin compounds

L6 ANSWER 22 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI The protease inhibitor p-nitrophenyl-p'-guanidinobenzoate inactivates Sindbis and other enveloped viruses

L6 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI 6-[.alpha.-(.omega.-Guanidinoalkanoylamido)acylamido]penicillanic acids

L6 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI 6-[.alpha.-(.omega.-Guanidinoalkanoylamido)acylamido]penicillanic acids

L6 ANSWER 25 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Influence of various proteinase inhibitors on the gelatinolytic effect of ejaculated and uterine boar spermatozoa

L6 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Pharmaceutical cephalosporins

L6 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Antimicrobial and hypoglycemic (2-imidazolidinylidene)- and (hexahydro-2-pyrimidinylidene)guanidines

L6 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Specificity and mechanism of clostripain catalysis

L6 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI **Antibacterial** guanidinoarylpenicillins

L6 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Tuberculostatic activity of derivatives of aminoguanidine and diaminoguanidine and its correlation with chemical structure

L6 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2003 ACS
TI Reaction of cyanoguanidine with aromatic amines. II. Formation of 1-amidino-3-(p-nitrophenyl- and p-carboxyphenyl)urea

=> pylori
7936 PYLORI
20 PYLORIS
L7 7949 PYLORI
(PYLORI OR PYLORIS)

=> l4 and l7
L8 2 L4 AND L7

=> d l8 1-2 ti

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
TI Preparation of esters of 4-guanidinyl(methyl)benzoic acid treating or preventing bacterial infection

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS
TI Enzyme inhibitors for treatment of gastrointestinal disorders caused by Helicobacter **pylori**

=> d l8 1-2 ti fbib abs

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
TI Preparation of esters of 4-guanidinyl(methyl)benzoic acid treating or preventing bacterial infection
AN 2003:282526 CAPLUS
DN 138:304065
TI Preparation of esters of 4-guanidinyl(methyl)benzoic acid treating or preventing bacterial infection
IN Zhu, Dexu; Muramatsu, Mutsumi; Xie, Jianshu; Cheng, Ni; Wang, Mingwei
PA Peop. Rep. China
SO PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003029201	A1	20030410	WO 2001-CN1499	20011023

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CN 2001-142289 A 20010926
CN 1410419 A 20030416 CN 2001-142289 20010926

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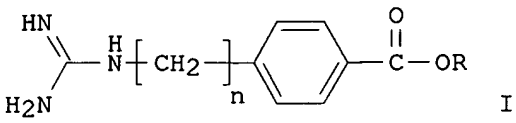


I

AB Title compds. I [n = 0-1; R = H, alkyl, aryl, biphenyl deriv.] are prepd. For instance, a suspension of 4-guanidinomethylbenzoic acid hydrochloride (prepn. given) is condensed with phenol (pyridine, DCC, 48 h) to give Ph 4-guanidinomethylbenzoate hydrochloride. Selected analogs had IC50 of >200 - 26 .mu.M on E. coli growth. Another example compd. had MIC of 0.10 - 0.48 .mu.g/mL against 9 strains of H. **pylori** at various pH. I are useful for treating or preventing disease or disorders caused by or assocd. with certain bacterial infection, esp. Escherichia coli (E. coli) or Helicobacter **pylori** (H. **pylori**) infection.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS
TI Enzyme inhibitors for treatment of gastrointestinal disorders caused by Helicobacter **pylori**
AN 1994:587325 CAPLUS
DN 121:187325
TI Enzyme inhibitors for treatment of gastrointestinal disorders caused by Helicobacter **pylori**
IN Wabnitz, Rudolf; Riedl, Jutta; Ansorg, Rainer; Goebell, Harald
PA Asche AG, Germany
SO Ger. Offen., 3 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 4305536	A1	19940825	DE 1993-4305536	19930219
WO 9418964	A1	19940901	WO 1994-EP523	19940218
W: AU, CA, FI, HU, JP, NO, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
			DE 1993-4305536A	19930219
AU 9462053	A1	19940914	AU 1994-62053	19940218
			DE 1993-4305536A	19930219
			WO 1994-EP523 W	19940218
EP 804184	A1	19971105	EP 1994-909036	19940218
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
			DE 1993-4305536A	19930219
			WO 1994-EP523 W	19940218
JP 2002515002	T2	20020521	JP 1994-518670	19940218
			DE 1993-4305536A	19930219
			WO 1994-EP523 W	19940218
WO 9614068	A1	19960517	WO 1994-EP3669	19941107

W: AT, CA, FI, HU, JP, NO, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
DE 1993-4305536 19930219

AB Enzyme inhibitors, esp. protease inhibitors such as .omega.-guanidinocarboxylic acid esters, are useful for treatment of H. **pylori**-assocd. gastrointestinal disorders. Thus, soft gelatin capsules contained camostat 100.00, soybean lecithin 5.00, 2,6-di-tert-butyl-4-methylphenol (antioxidant) 0.1, and peanut oil to 800.00 mg.

=> d l8 2 it

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

IT Carboxylic acids, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(guanidino, esters, Helicobacter **pylori**-assocd. digestive disorder treatment with)

IT Campylobacter pyloridis
(infection with, digestive disorder from, treatment of, with proteinase inhibitors)

IT Enzymes
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors, Helicobacter **pylori**-assocd. digestive disorder treatment with)

IT Digestive tract
(disease, infection, with Helicobacter **pylori**, treatment of, with proteinase inhibitors)

IT Onium compounds
RL: BIOL (Biological study)
(guanidinium, carboxy, Helicobacter **pylori**-assocd. digestive disorder treatment with)

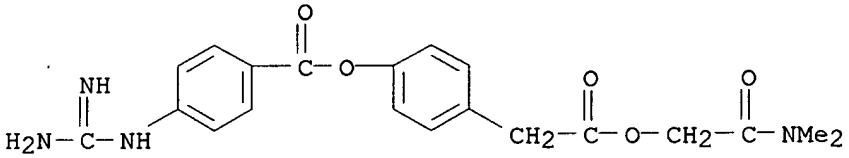
IT 6659-35-4D, .epsilon.-Guanidinocaproic acid, esters **16060-65-4D**, p-Guanidinobenzoic acid, esters 37205-61-1, Proteinase inhibitor 39492-01-8, Gabexate **59721-28-7**, Camostat **71079-09-9**, FOY 251 **81525-10-2**, Nafamostat
RL: BIOL (Biological study)
(Helicobacter **pylori**-assocd. digestive disorder treatment with)

=> 59721-28-7
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

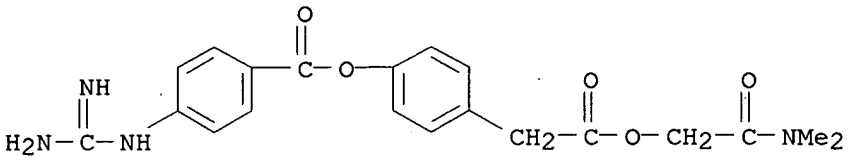
L10 82 L9

=> display hitstr
ENTER (L10), L# OR ?:l10
ENTER ANSWER NUMBER OR RANGE (1):1-5

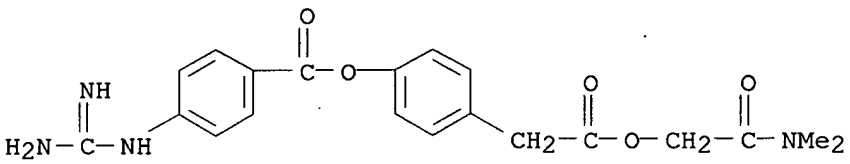
L10 ANSWER 1 OF 82 CAPLUS COPYRIGHT 2003 ACS
IT **59721-28-7,** Camostat
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(development of camostat mesilate troche for prevention of mucositis in
mouth during cancer chemotherapy (Erratum))
RN 59721-28-7 CAPLUS
CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-, 2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



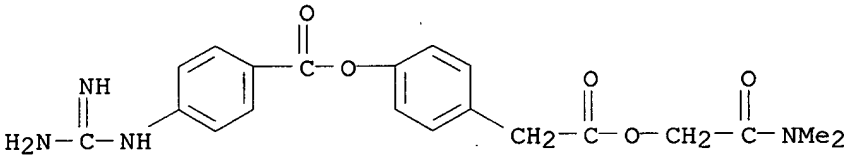
L10 ANSWER 2 OF 82 CAPLUS COPYRIGHT 2003 ACS
IT **59721-28-7,** Camostat
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(trypsin inhibitor camostat has different effects on pancreas between cholecystokinin-A receptor gene knockout and wild-type mice)
RN 59721-28-7 CAPLUS
CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-, 2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



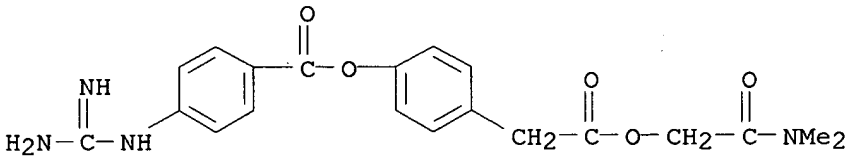
L10 ANSWER 3 OF 82 CAPLUS COPYRIGHT 2003 ACS
IT **59721-28-7,** Camostat
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(metabolite; development of camostat mesilate troche for prevention of mucositis in mouth during cancer chemotherapy)
RN 59721-28-7 CAPLUS
CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-, 2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 4 OF 82 CAPLUS COPYRIGHT 2003 ACS
IT **59721-28-7**
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(fish feed contg. proteinase inhibitors)
RN 59721-28-7 CAPLUS
CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,
2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 5 OF 82 CAPLUS COPYRIGHT 2003 ACS
IT **59721-28-7**, Camostat
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
THU
(Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(prepn. and characterization of biodegradable or enteric-coated
microspheres contg. the protease inhibitor camostat)
RN 59721-28-7 CAPLUS
CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,
2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.16	179.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.30

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 12:40:34 ON 03 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1623paz

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 12:42:25 ON 03 JUN 2003
FILE 'CAPLUS' ENTERED AT 12:42:25 ON 03 JUN 2003
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.16	179.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.30

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.58	179.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.30

FILE 'REGISTRY' ENTERED AT 12:42:50 ON 03 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2
DICTIONARY FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

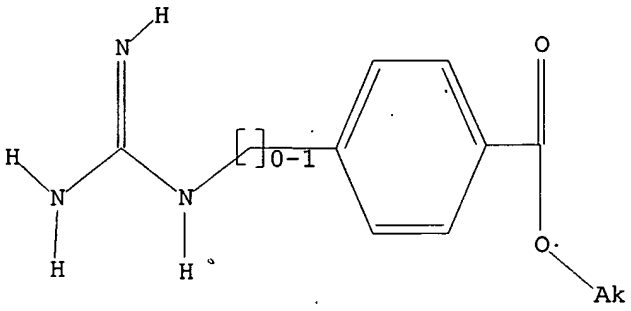
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties

in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 09975136 before allowance.str

L11 STRUCTURE UPLOADED

=> d l11
L11 HAS NO ANSWERS
L11 STR



G1 H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> search l11 sss sam
SAMPLE SEARCH INITIATED 12:43:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 208 TO ITERATE

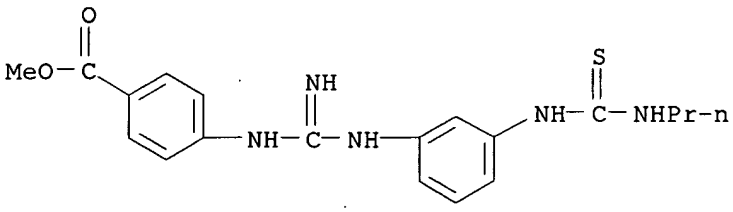
100.0% PROCESSED 208 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3295 TO 5025
PROJECTED ANSWERS: 9 TO 360

L12 9 SEA SSS SAM L11

=> d scan

L12 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, p-[3-[m-(3-propyl-2-thioureido)phenyl]guanidino]-, methyl ester, monohydrochloride (8CI)
MF C19 H23 N5 O2 S . Cl H



● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>
=>
Uploading 09975136 before allowance.str

L13 STRUCTURE UPLOADED

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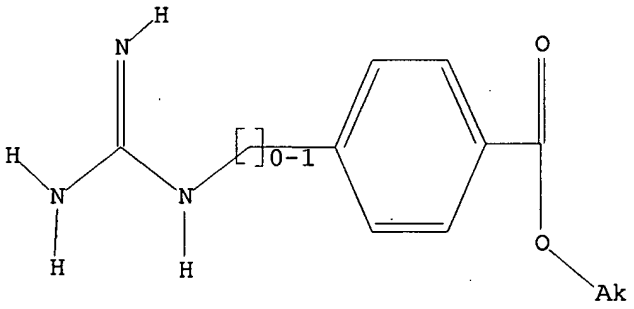
L13 HAS NO ANSWERS
L13 STR



G1 H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 208 TO ITERATE

100.0% PROCESSED 208 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

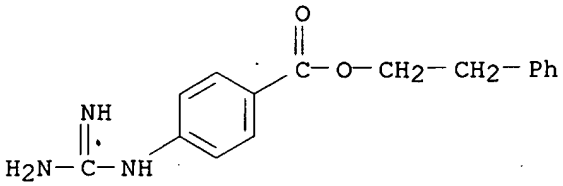
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3295 TO 5025
PROJECTED ANSWERS: 9 TO 360

L14 9 SEA SSS SAM L13

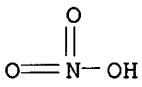
=> d scan

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-phenylethyl ester, mononitrate (9CI)
MF C16 H17 N3 O2 . H N O3

CM 1

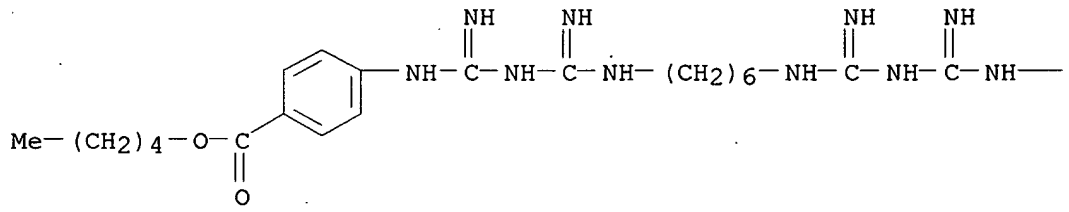


CM 2

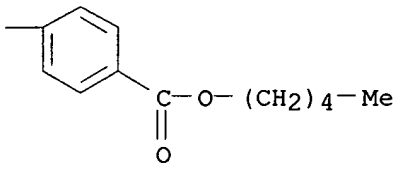


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

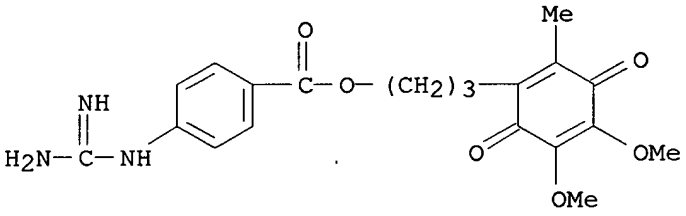
L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4,4'-[(1,3,12,14-tetraimino-2,4,11,13-tetraazatetradecane-1,14-diyl)diimino]bis-, dipentyl ester, dihydrochloride (9CI)
MF C34 H52 N10 O4 . 2 Cl H



●2 HCl

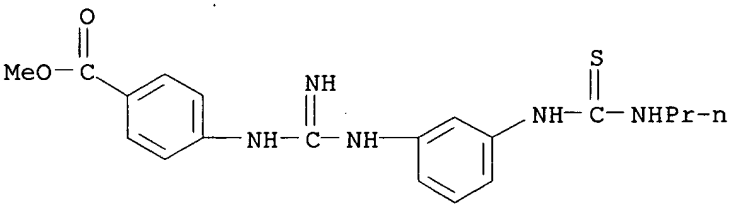


L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 3-(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)propyl ester (9CI)
MF C20 H23 N3 O6



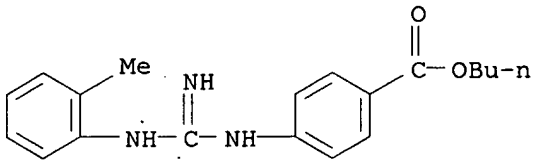
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, p-[3-[m-(3-propyl-2-thioureido)phenyl]guanidino]-, methyl ester, monohydrochloride (8CI)
MF C19 H23 N5 O2 S . Cl H



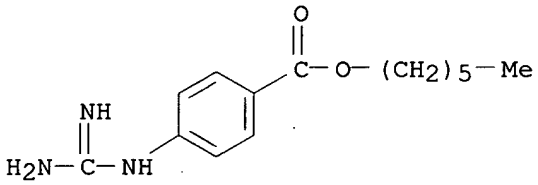
● HCl

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[imino[(2-methylphenyl)amino]methyl]amino]-, butyl ester (9CI)
MF C19 H23 N3 O2



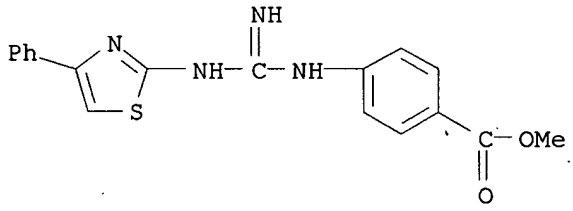
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, hexyl ester (9CI)
MF C14 H21 N3 O2
CI COM



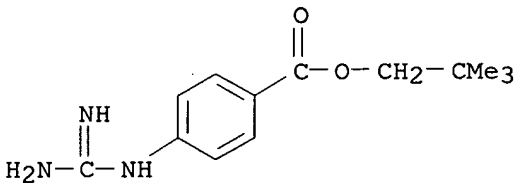
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[imino[(4-phenyl-2-thiazolyl)amino]methyl]amino]-, methyl
ester (9CI)
MF C18 H16 N4 O2 S



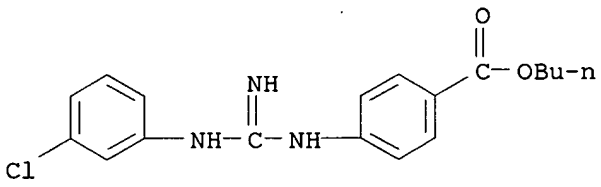
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester (9CI)
MF C13 H19 N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[[(3-chlorophenyl)amino]iminomethyl]amino]-, butyl ester (9CI).
MF C18 H20 Cl N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester/cn
E1 1 BENZOIC ACID,
4,6-DIMETHOXY-3-(5-METHOXY-2-(METHOXYCARBONYL)
-3-PENTYLPHENOXY)-2-PENTYL-, METHYL ESTER/CN
E2 1 BENZOIC ACID, 4,6-DIMETHOXY-3-METHYL-2-(1-OXOBUTOXY)-,
METHY
L ESTER/CN
E3 0 --> BENZOIC ACID, 4-(AMINOIMINOMETHYL)AMINO-, 2,2-DIMETHYLPROP
YL ESTER/CN
E4 1 BENZOIC ACID,
4-((((((((2,3-DIHYDRO-2,2-DIMETHYL-7-BENZOFURA

```
NYL)OXY)CARBONYL)METHYLAMINO)CARBONYL)AMINO)SULFONYL)AMINO)-
                    , ETHYL ESTER/CN
E5          1       BENZOIC ACID,
4-(((((((2,3,4-TRICHLOROPHENYL)THIO)ACETYL)OXY
                    )ACETYL)AMINO)METHYL)-, METHYL ESTER/CN
E6          1       BENZOIC ACID,
4-(((((((3.BETA.)-17-OXOANDROST-5-EN-3-YL)AMIN
                    O)CARBONYL)OXY)METHYL)AMINO)-, 2-(DIETHYLAMINO)ETHYL
ESTER/C
                    N
E7          1       BENZOIC ACID,
4-(((((((3.BETA.)-17-OXOANDROST-5-EN-3-YL)OXY)
                    METHYL)THIO)METHYL)AMINO)-, 2-(DIMETHYLAMINO)ETHYL ESTER/CN
E8          1       BENZOIC ACID,
4-(((((((3.BETA.,17.BETA.)-3-HYDROXYANDROST-5-
                    EN-17-YL)AMINO)CARBONYL)OXY)METHYL)AMINO)-,
2-(DIETHYLAMINO)
                    ETHYL ESTER/CN
E9          1       BENZOIC ACID,
4-(((((((4-BROMO-8-CHLORO-1-NAPHTHALENYL)THIO)
                    ACETYL)OXY)ACETYL)AMINO)METHYL)-, METHYL ESTER/CN
E10         1       BENZOIC ACID,
4-(((((((4-CHLOROPHENYL)AMINO)CARBONYL)HYDRAZO
                    NO)PHENYLMETHYL)THIO)METHYL)-, 1,1-DIMETHYLETHYL ESTER/CN
E11         1       BENZOIC ACID,
4-(((((((4-CHLOROPHENYL)SULFONYL)AMINO)PHENYLM
                    ETHYLENE)AMINO)THIOXOMETHYL)AMINO)-/CN
E12         1       BENZOIC ACID,
4-(((((((4-METHOXYPHENYL)SULFONYL)(PHENYLMETHY
                    L)AMINO)ACETYL)AMINO)OXY)DIPHENYLMETHYL)-/CN

=> e Benzoic acid, 4-((aminoiminomethyl)amino)-, 2,2-dimethylpropyl ester/cn
E1          1       BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-, 1-NAPHTHALENYL
E
                    STER, METHANESULFONATE/CN
E2          1       BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-, 1-NAPHTHALENYL
E
                    STER, MONONITRATE/CN
E3          1 --> BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,2-DIMETHYLPROP
                    YL ESTER/CN
E4          1       BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,3-DIFLUOROPHEN
                    YL ESTER/CN
E5          1       BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,3-DIFLUOROPHEN
                    YL ESTER, MONOACETATE/CN
E6          1       BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,3-DIMETHOXYPHE
                    NYL ESTER, MONOHYDROCHLORIDE/CN
E7          1       BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,3-DIMETHYLPHEN
                    YL ESTER/CN
E8          1       BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,3-DIMETHYLPHEN
                    YL ESTER, MONOMETHANESULFONATE/CN
E9          1       BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,4-DINITROPHENY
```

```
                    L ESTER/CN
E10          1      BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,5-DICHLOROPHEN
                    YL ESTER/CN
E11          1      BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,5-DICHLOROPHEN
                    YL ESTER, MONOMETHANESULFONATE/CN
E12          1      BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,6-DICHLORO-4-N
                    ITROPHENYL ESTER/CN

=> e3
L15          1 "BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,
2,2-DIMETHYLPROPYL
               ESTER"/CN

=> d l15

L15  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS
RN   282718-30-3  REGISTRY
CN   Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester
     (9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C13 H19 N3 O2
SR   CA
LC   STN Files:   CA, CAPLUS
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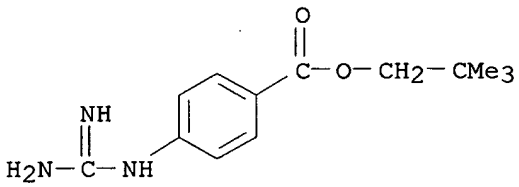


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

              1 REFERENCES IN FILE CA (1957 TO DATE)
              1 REFERENCES IN FILE CAPLUS (1957 TO DATE)


=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     8.70     188.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -1.30

FILE 'CAPLUS' ENTERED AT 12:46:56 ON 03 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 3 Jun 2003 VOL 138 ISS 23
FILE LAST UPDATED: 2 Jun 2003 (20030602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l15
L16 1 L15

=> d l16 ti fbib abs

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
TI (4-aminomethyl)phenylguanidine derivatives as nonpeptidic highly selective
inhibitors of human urokinase
AN 2000:341443 CAPLUS
DN 133:99075
TI (4-aminomethyl)phenylguanidine derivatives as nonpeptidic highly selective
inhibitors of human urokinase
AU Sperl, Stefan; Jacob, Uwe; De Prada, Nuria Arroyo; Sturzebecher, Jorg; Wilhelm, Olaf G.; Bode, Wolfram; Magdolen, Viktor; Huber, Robert; Moroder,
Luis
CS Max-Planck-Institut fur Biochemie, Martinsried, 82152, Germany
SO Proceedings of the National Academy of Sciences of the United States of America (2000), 97(10), 5113-5118
CODEN: PNASA6; ISSN: 0027-8424
PB National Academy of Sciences
DT Journal
LA English
AB Increased expression of the serine protease urokinase-type plasminogen activator (uPA) in tumor tissues is highly correlated with tumor cell migration, invasion, proliferation, progression, and metastasis. Thus inhibition of uPA activity represents a promising target for antimetastatic therapy. So far, only the x-ray crystal structure of uPA inactivated by H-Glu-Gly-Arg-chloromethylketone has been reported, thus limited data are available for a rational structure-based design of uPA inhibitors. Taking into account the trypsin-like arginine specificity of uPA, (4-aminomethyl)phenylguanidine was selected as a potential P1 residue
and iterative derivatization of its amino group with various hydrophobic residues, and structure-activity relationship-based optimization of the spacer in terms of hydrogen bond acceptor/donor properties led to N-(1-adamantyl)-N'-(4-guanidinobenzyl)urea as a highly selective

nonpeptidic uPA inhibitor. The x-ray crystal structure of the uPA B-chain
complexed with this inhibitor revealed a surprising binding mode consisting of the expected insertion of the phenylguanidine moiety into the S1 pocket, but with the adamantyl residue protruding toward the hydrophobic S1' enzyme subsite, thus exposing the ureido group to hydrogen-bonding interactions. Although in this enzyme-bound state the inhibitor is crossing the active site, interactions with the catalytic residues Ser-195 and His-57 are not obsd., but their side chains are spatially displaced for steric reasons. Compared with other trypsin-like serine proteases, the S2 and S3/S4 pockets of uPA are reduced in size because of the 99-insertion loop. Therefore, the peculiar binding mode of
the new type of uPA inhibitors offers the possibility of exploiting optimized interactions at the 51'/S2' subsites to further enhance selectivity and potency. Because crystals of the uPA/benzamidine complex allow inhibitor exchange by soaking procedures, the structure-based design
of new generations of uPA inhibitors can rely on the assistance of x-ray anal.
RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.50	192.90

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.65	-1.95

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 12:50:12 ON 03 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1623paz

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	Jun 03	New e-mail delivery for search results now available
NEWS	4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS	5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS	6	Aug 26	Sequence searching in REGISTRY enhanced

NEWS 7 Sep 03 JAPIO has been reloaded and enhanced
NEWS 8 Sep 16 Experimental properties added to the REGISTRY file
NEWS 9 Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 10 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11 Oct 24 BEILSTEIN adds new search fields
NEWS 12 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13 Nov 18 DKILIT has been renamed APOLLIT
NEWS 14 Nov 25 More calculated properties added to REGISTRY
NEWS 15 Dec 04 CSA files on STN
NEWS 16 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17 Dec 17 TOXCENTER enhanced with additional content
NEWS 18 Dec 17 Adis Clinical Trials Insight now available on STN
NEWS 19 Jan 29 Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20 Feb 13 CANCERLIT is no longer being updated
NEWS 21 Feb 24 METADEX enhancements
NEWS 22 Feb 24 PCTGEN now available on STN
NEWS 23 Feb 24 TEMA now available on STN
NEWS 24 Feb 26 NTIS now allows simultaneous left and right truncation
NEWS 25 Feb 26 PCTFULL now contains images
NEWS 26 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27 Mar 20 EVENTLINE will be removed from STN
NEWS 28 Mar 24 PATDPAFULL now available on STN
NEWS 29 Mar 24 Additional information for trade-named substances without structures available in REGISTRY
NEWS 30 Apr 11 Display formats in DGENE enhanced
NEWS 31 Apr 14 MEDLINE Reload
NEWS 32 Apr 17 Polymer searching in REGISTRY enhanced
NEWS 33 Apr 21 Indexing from 1947 to 1956 being added to records in CA/CAPLUS
NEWS 34 Apr 21 New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 35 Apr 28 RDISCLOSURE now available on STN
NEWS 36 May 05 Pharmacokinetic information and systematic chemical names added to PHAR
NEWS 37 May 15 MEDLINE file segment of TOXCENTER reloaded
NEWS 38 May 15 Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39 May 16 CHEMREACT will be removed from STN
NEWS 40 May 19 Simultaneous left and right truncation added to WSCA
NEWS 41 May 19 RAPRA enhanced with new search field, simultaneous left and right truncation
NEWS 42 Jun 06 Simultaneous left and right truncation added to CBNB
NEWS 43 Jun 06 PASCAL enhanced with additional data

NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
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NEWS INTER General Internet Information
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

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